

# Development of a New Unresolved Resonance Region Analysis Methodology

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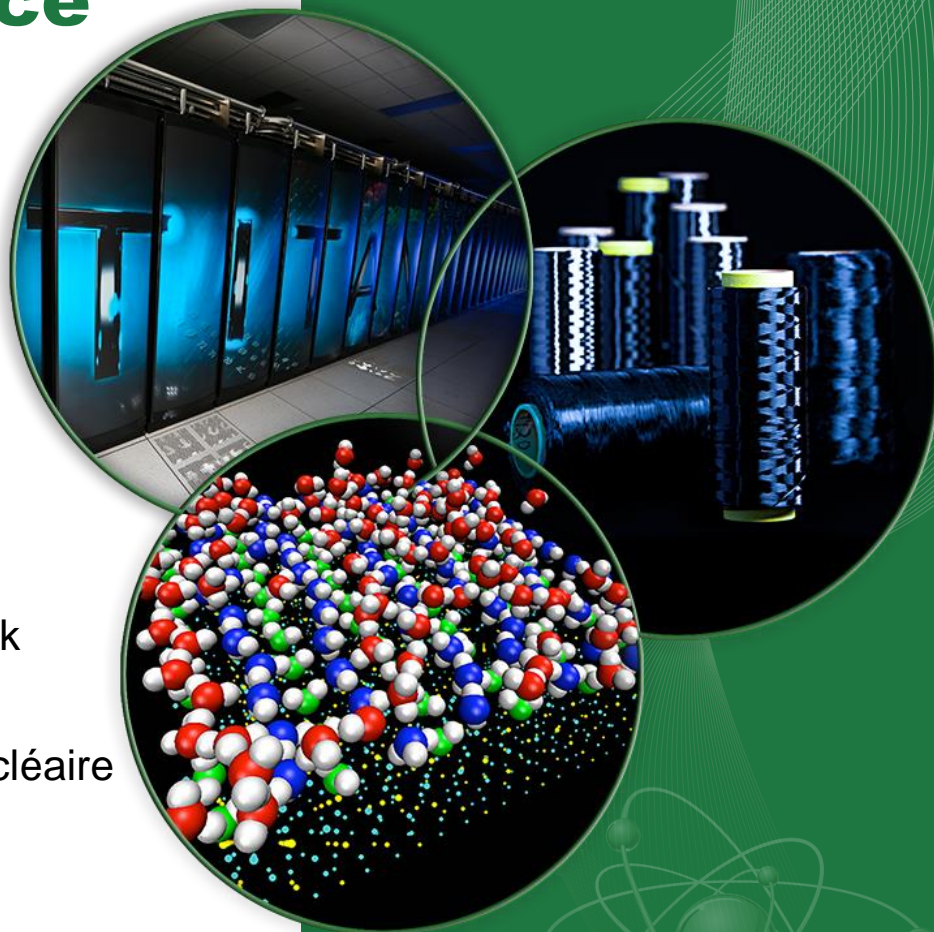
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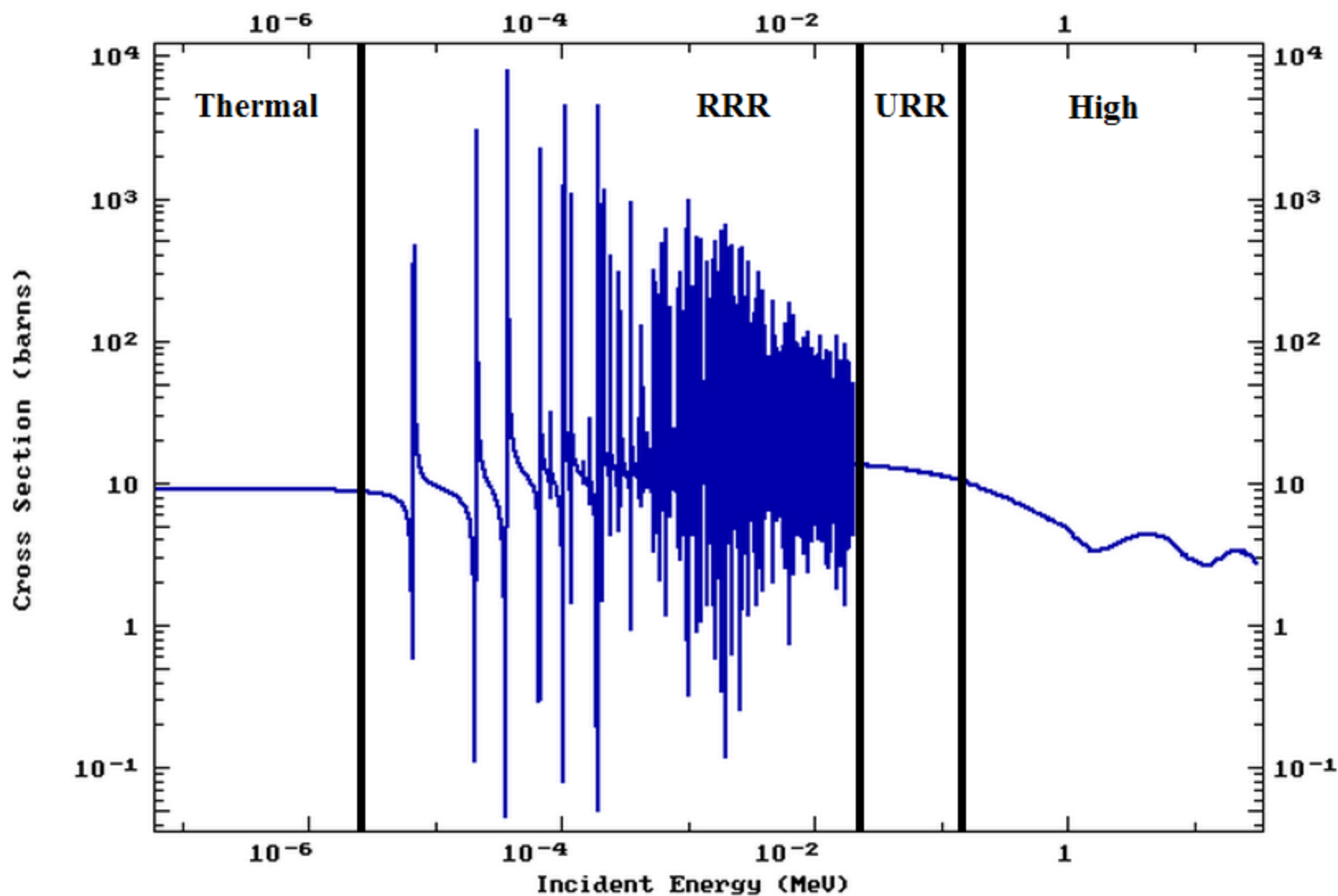
# Outline

- Objective
- Background
- New Unresolved Resonance Region Methodology
- Results
  - Resolved Resonance Region (RRR)
    - Test Cases: Energy-Differential and Double-Differential XS's in RRR for  $^{16}\text{O}$ ,  $^{19}\text{F}$ ,  $^{35}\text{Cl}$ ,  $^{56}\text{Fe}$ ,  $^{63}\text{Cu}$ ,  $^{65}\text{Cu}$
  - Unresolved Resonance Region (URR)
    - Updated  $^{238}\text{U}$  cross section probability tables
    - International Criticality Safety Benchmark Evaluation Project (ICSBEP) benchmarks: IEU-COMP-FAST-004, IEU-MET-FAST-003, and IEU-MET-FAST-007
- Conclusions and Future Work

# Objective

- Create a modern implementation of the R-Matrix Limited algorithm
  - Help achieve goal of updating AMPX code to modern language (C++)
- Develop an unresolved resonance region (URR) analysis methodology consistent with the methodology used in the resolved resonance region (RRR)
  - Improve model fidelity for criticality safety and shielding problems

# $^{238}\text{U}$ Elastic Scattering Cross Section at 0K [1]



# Advantages of Reich-Moore Approximation

- Closest to full R-Matrix (too complex)
- Treats capture channels in an aggregate manner, but:
  - Allows multiple inelastic channels and charged particle channels, like (n,α), (n,p), etc
  - All other reactions take into account **channel-channel** and **level-level** interference:

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E} \delta_{JJ'}$$

# Temperature effects

- So far, equations only generate  $\sigma_x(E, T = 0)$ 
  - Temperature of media (not single nuclei) gives rise to distribution of velocities [3] :

$$v\sigma_{Doppler}(mv^2/2) \equiv \int d^3V p(\vec{V}) |\vec{v} - \vec{V}| \sigma(m|\vec{v} - \vec{V}|^2/2)$$

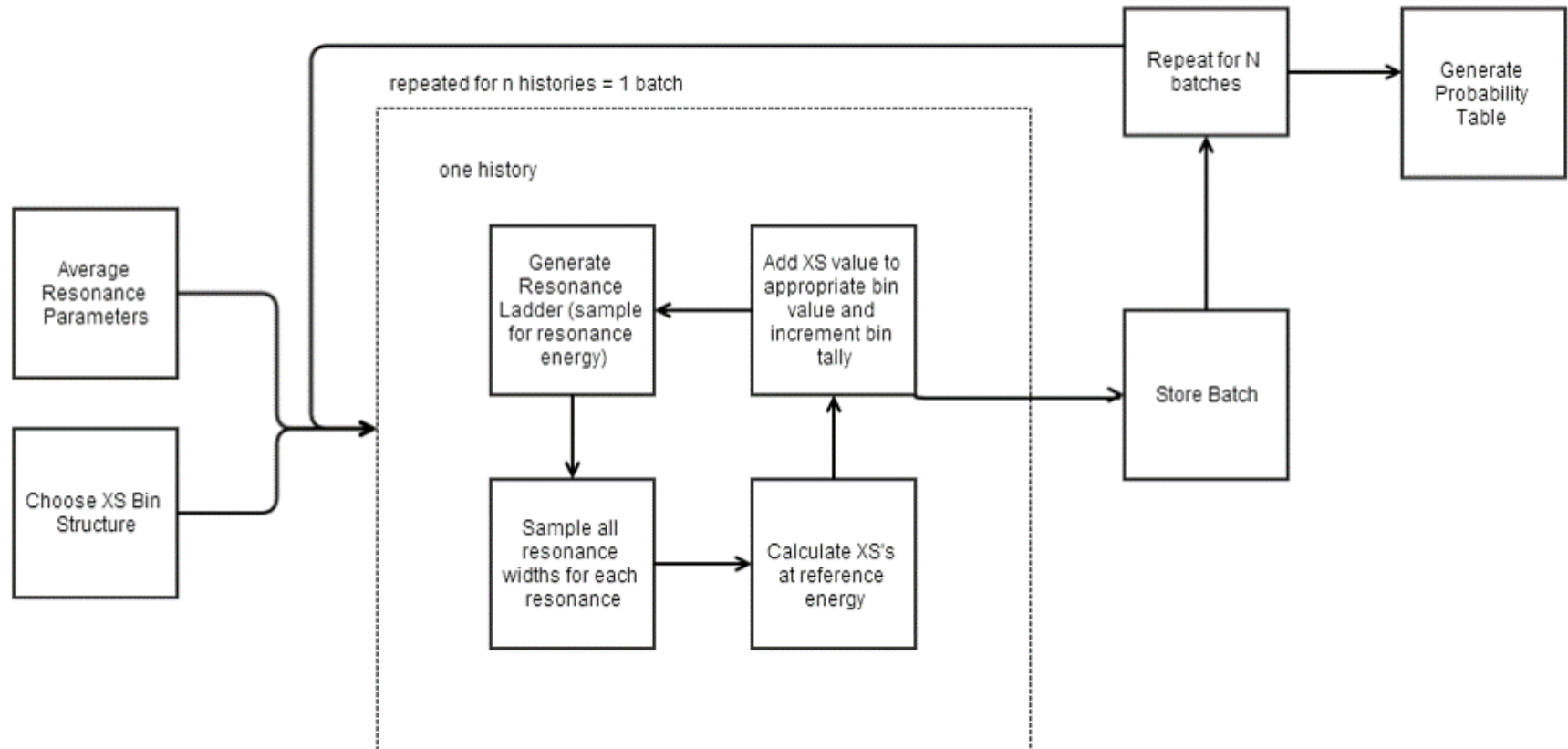
- $p(\vec{V})$  not known, assume Maxwell-Boltzmann distribution to get free-gas model:

$$\sigma_{Doppler}(mv^2/2) = \frac{1}{\sqrt{\pi}v^2 u} \int_0^\infty dr r^2 \sigma(mr^2/2) \left[ e^{-\left(\frac{v-r}{u}\right)^2} - e^{-\left(\frac{v+r}{u}\right)^2} \right]$$

# URR Cross Section Reconstruction

- Only have average parameter values, so XS's must be generated using a statistical sampling technique
  - Sample resonance level spacing around each energy of reference, sample resonance width of each reaction, then calculate XS at reference energy
    - Used to generate probability table for XS sampling during neutronics calculation
- Currently, only one cross section formalism is available... Single-Level Breit-Wigner

# URR Probability Table



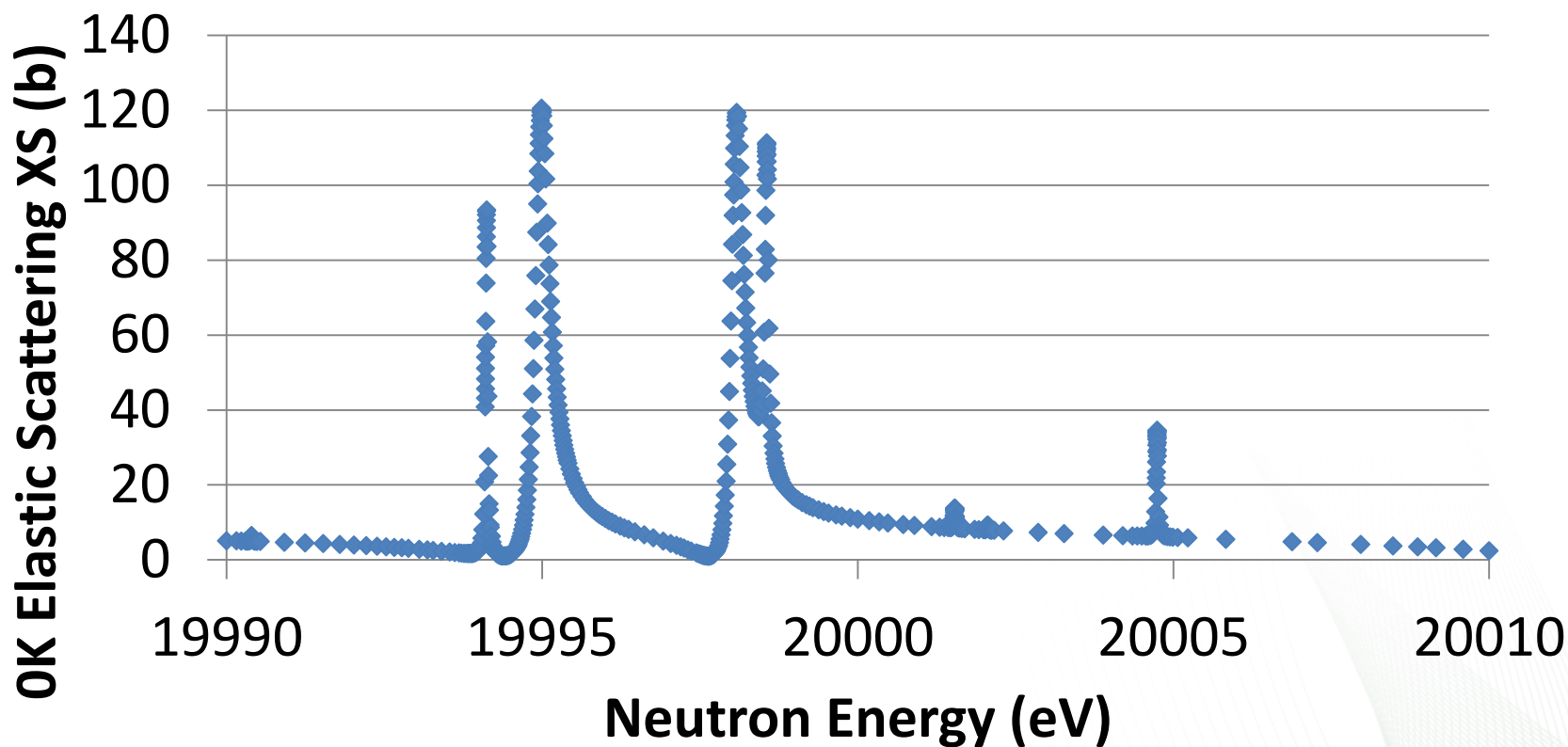
# New Unresolved Resonance Region Methodology

- Samples resonance spacing and widths in a way analogous to PURM (Wigner and Chi-Square distributions)
  - Generates Reich-Moore (RM) parameter set
    - Takes channel input from supplemental user input
    - Resamples for additional channels as necessary
  - Updates parameter sampling based on grid position
- Cross-Section calculation
  - SLBW approximation is replaced by the more robust RM formalism
  - Temperature broadening via Leal-Hwang method [6,7]
    - Requires energy grid [8]

# Example

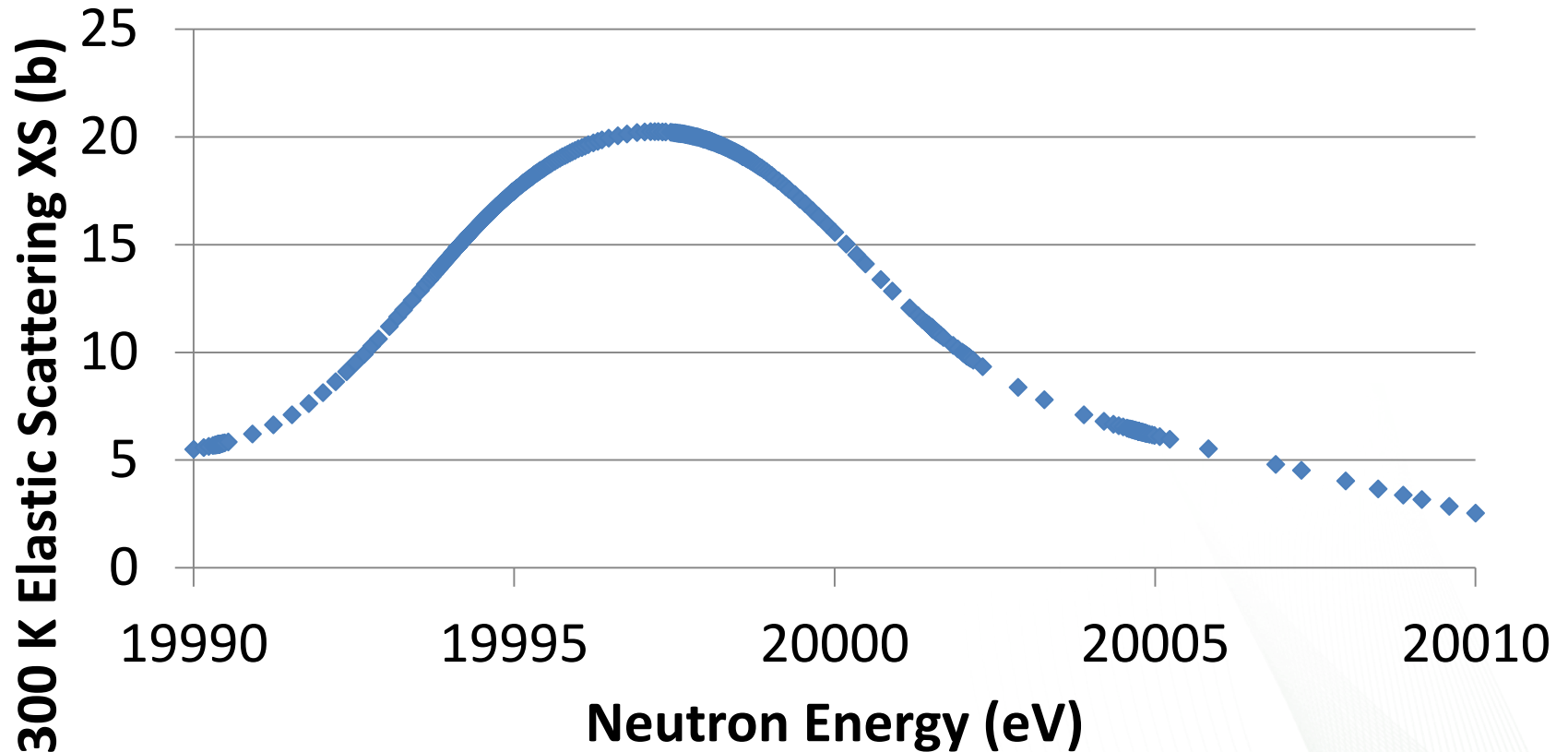
- Sample...

## $^{238}\text{U}$ Sample History Reconstruction - Unbroadened



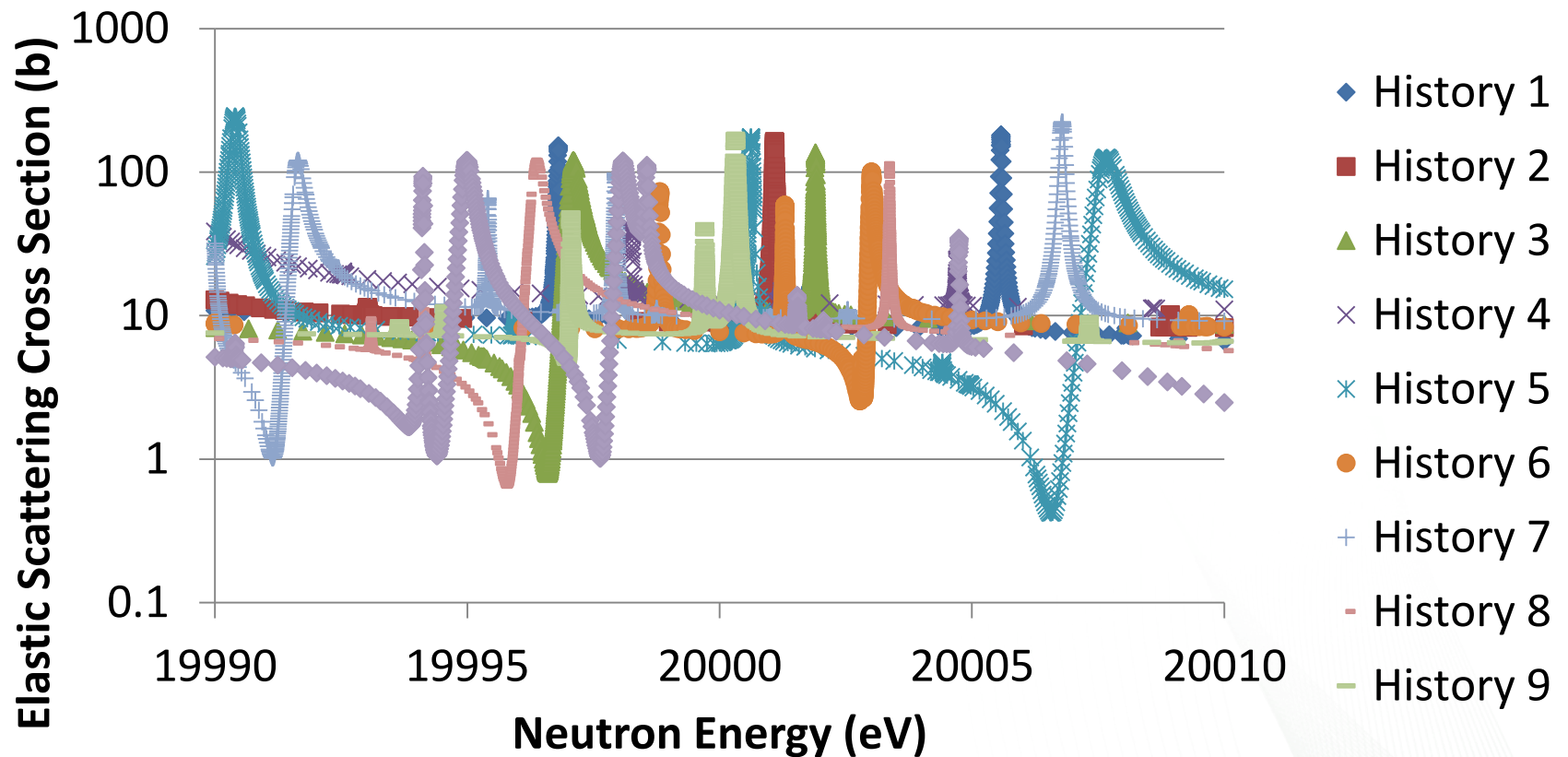
- Broaden...

## $^{238}\text{U}$ Sample History Reconstruction - Doppler Broadened



- Repeat many times...

## 238U Sample Batch



- Bin results, create probability table!

<b><math>^{238}\text{U}</math> Elastic Scattering XS at 20 keV, 300 K</b>			
<b>Bin</b>	Probability	XS (b)	$d\sigma$ (b)
<b>1</b>	0.2	9.61	1.04
<b>2</b>	0.2	11.43	0.39
<b>3</b>	0.2	12.87	0.46
<b>4</b>	0.2	14.84	0.72
<b>5</b>	0.2	20.46	4.24

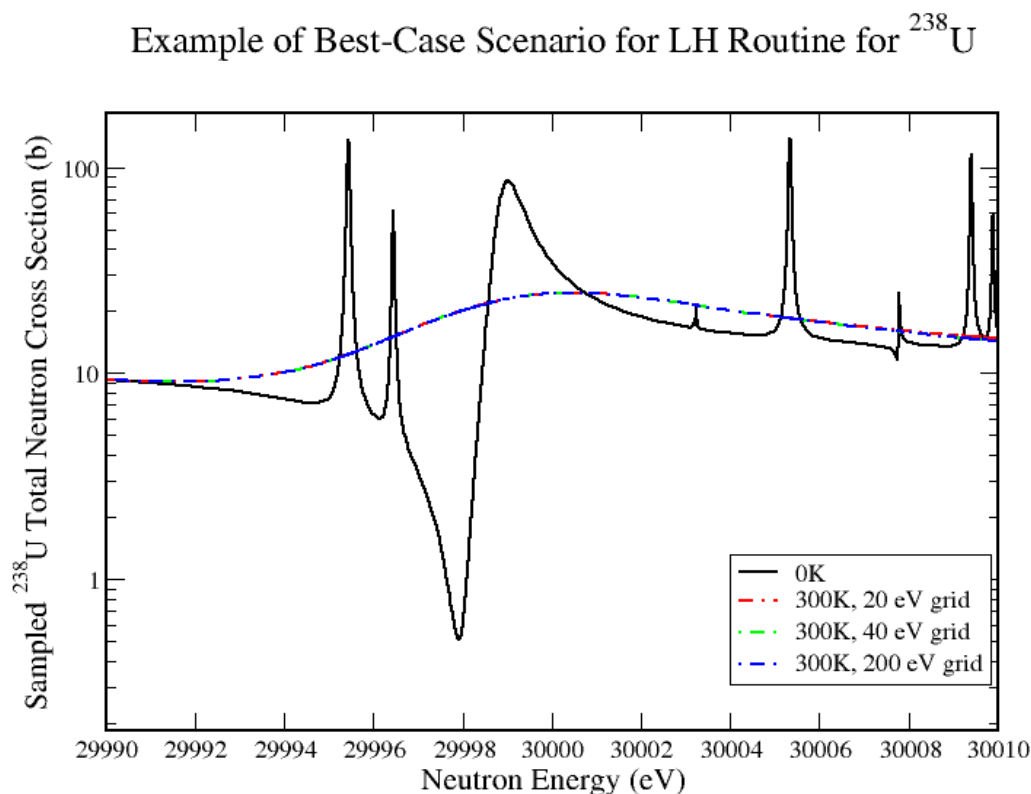
# Results – Resolved Resonance Region

- Tested new RML module by reconstructing energy-differential and double-differential cross sections for:
  - $^{16}\text{O}$  -  $(n, \alpha)$  reaction above 2.4 MeV
  - $^{19}\text{F}$  – two inelastic excitations in RRR
  - $^{35}\text{Cl}$  -  $(n, p)$  reaction with no threshold energy
  - $^{56}\text{Fe}$  – single inelastic reaction in RRR
  - $^{63}\text{Cu}$  and  $^{65}\text{Cu}$  – only elastic scattering and capture, different masses but same negative-parity ground state

# Results – Unresolved Resonance Region

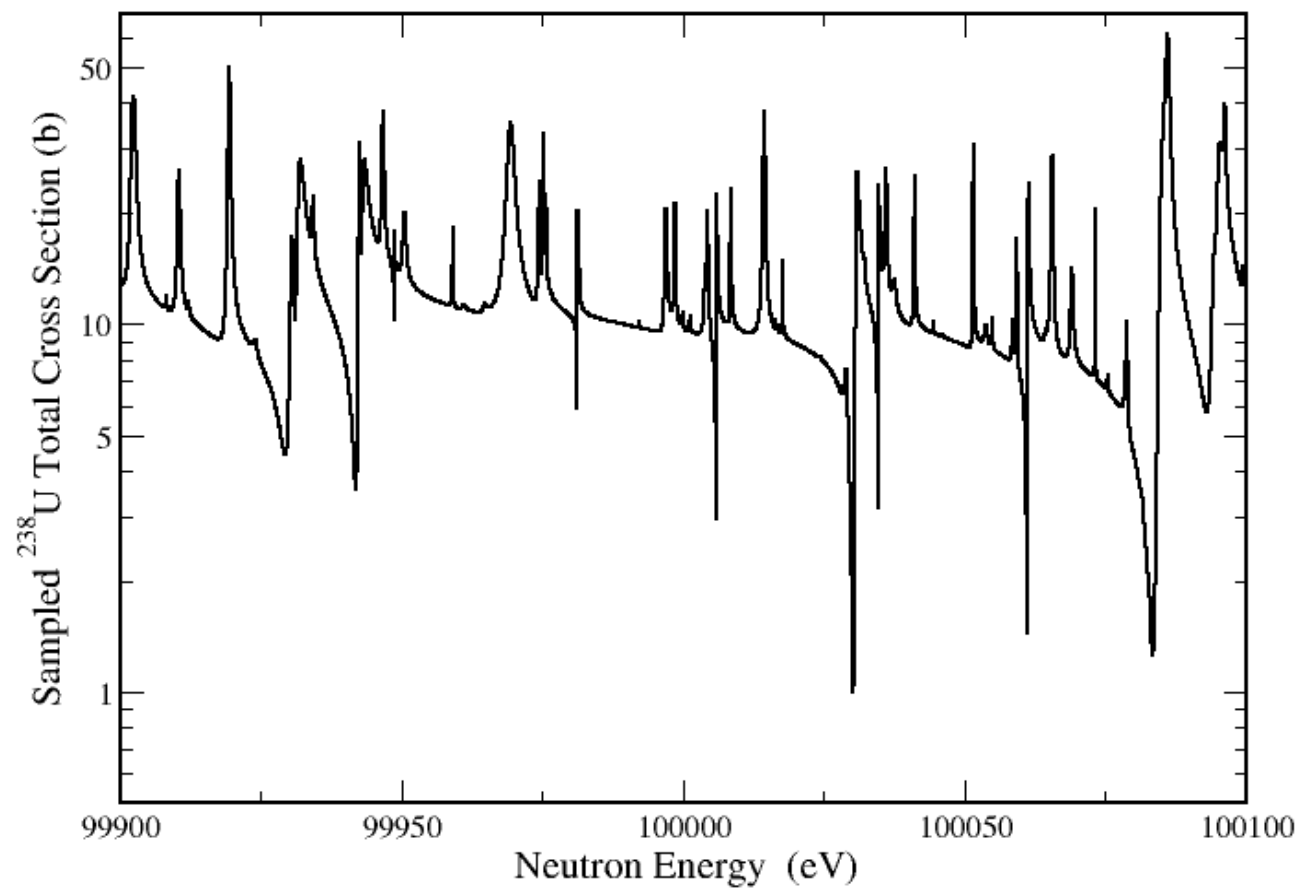
- Probability table generated for  $^{238}\text{U}$  for all energies of reference given in the ENDF file
  - Generated using both PURM and new method
    - PURM results
      - generated at 293.6 K
      - 60,000 histories
      - parameters sampled from  $E_{ref}$  only
    - New method results
      - generated at 293.6 K
      - 30,000 histories
      - parameters taken from nearest neighbor

- Grid justification...
  - RML formalism does not allow single-point broadening
  - Best-case scenario:

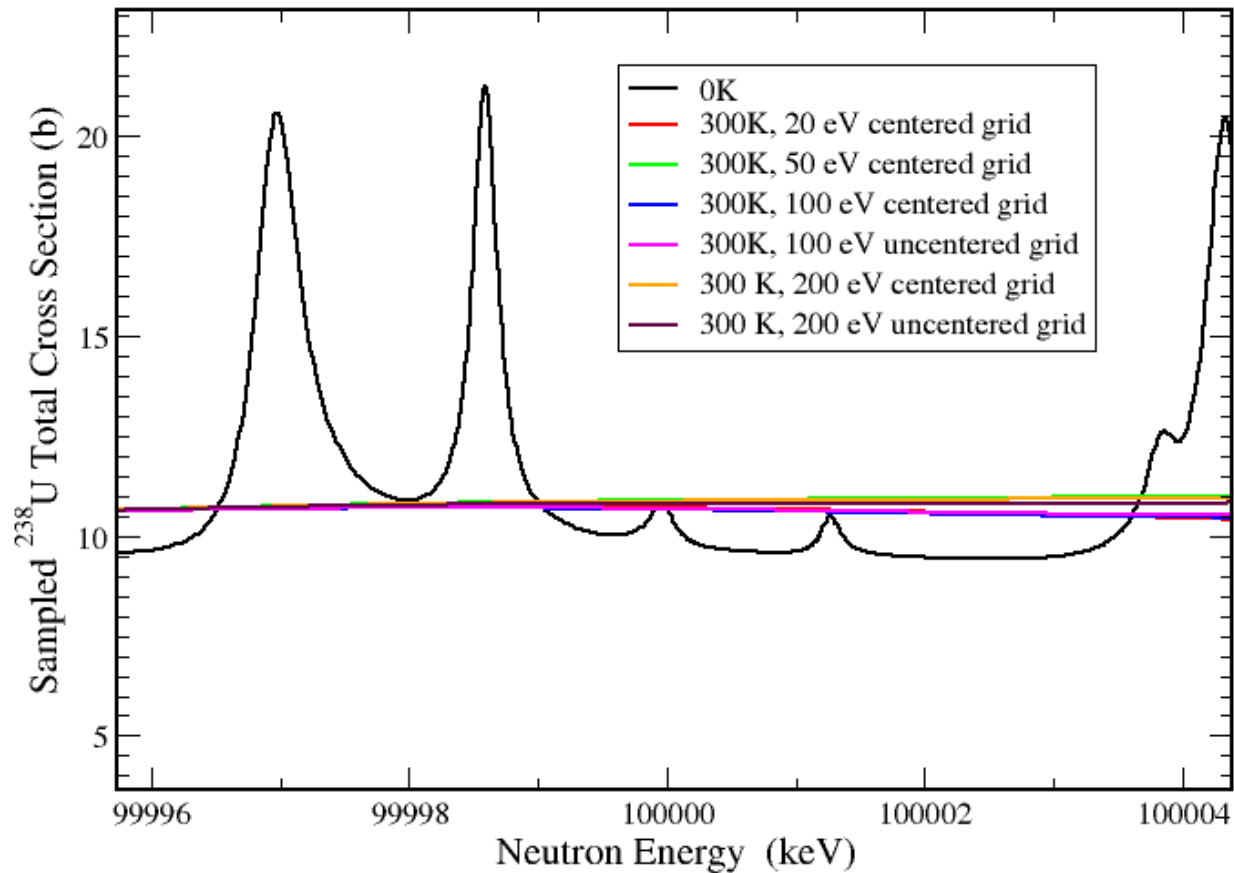


— Worst-case scenario:

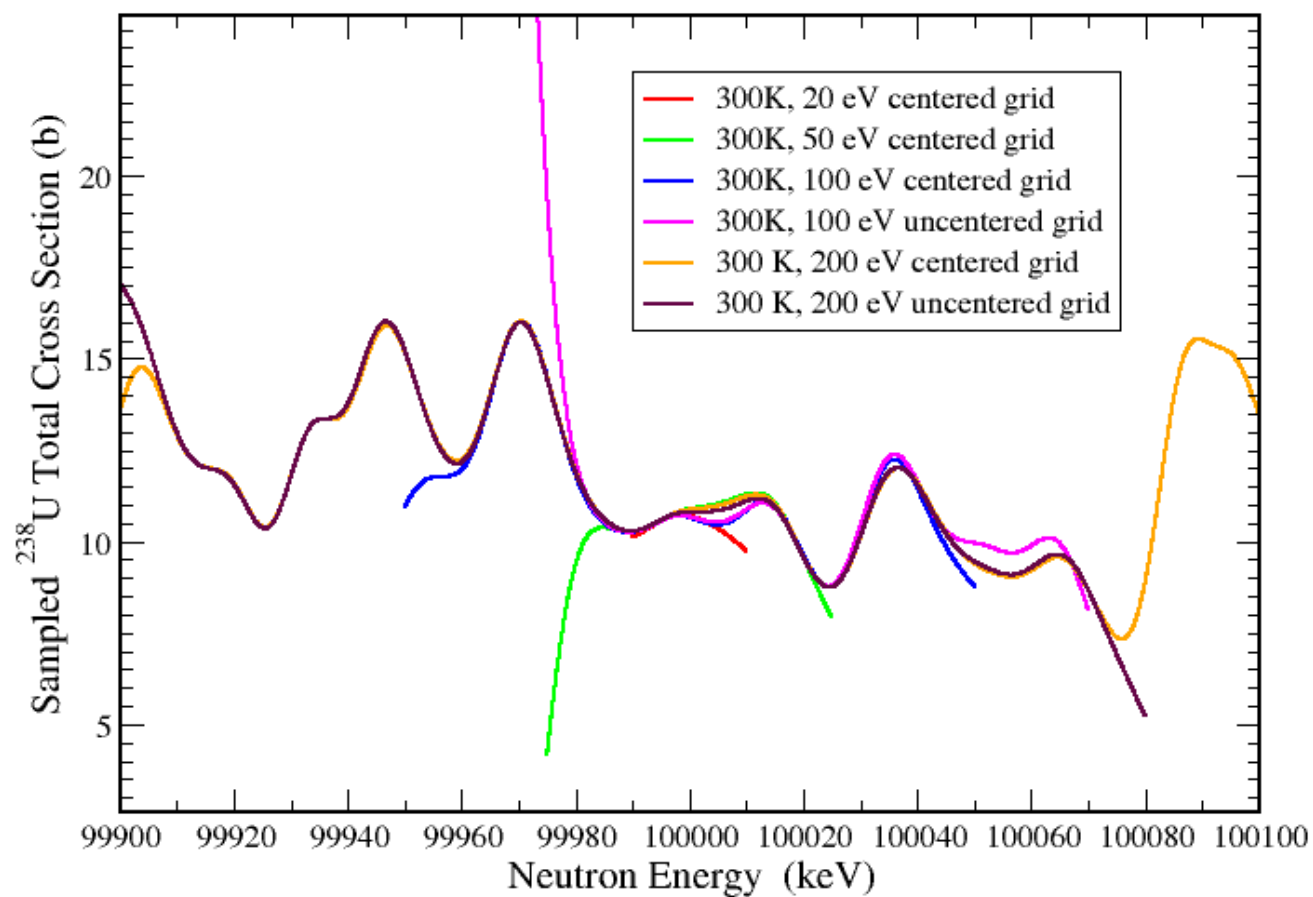
$^{238}\text{U}$  Total Cross Section at 0K for Worst-Case Broadening Scenario



## Worst-Case Broadening Scenario at $E_{\text{ref}}$

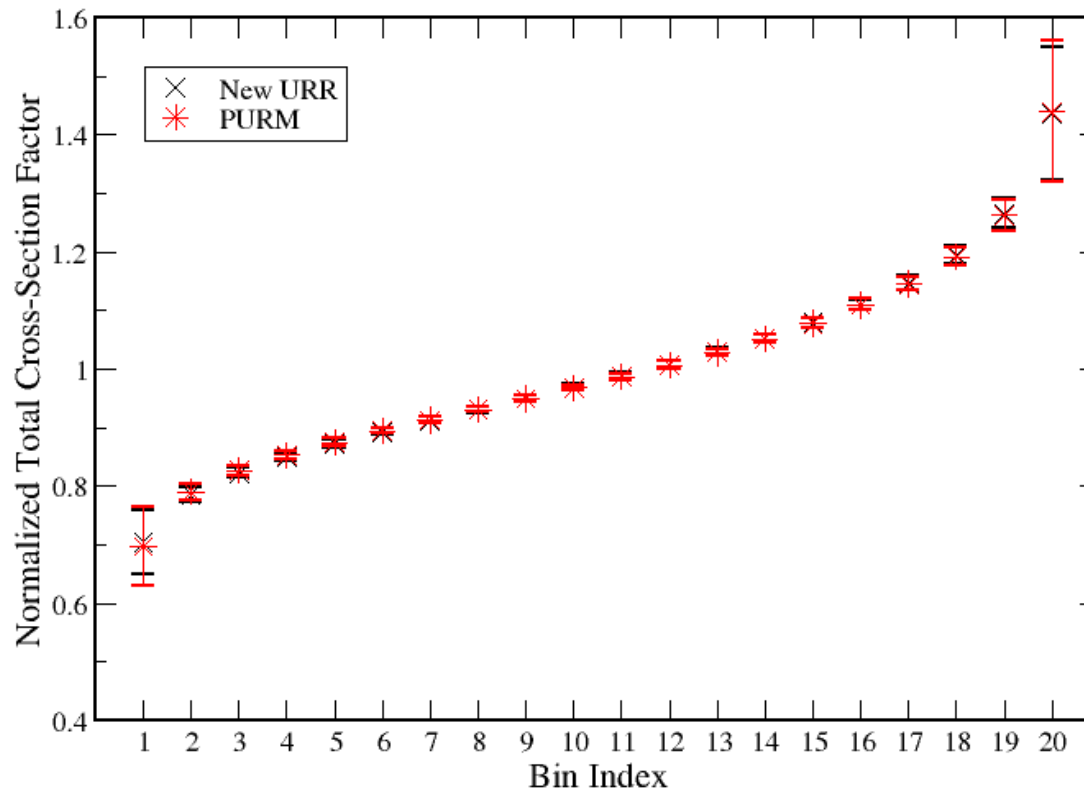


## Worst-Case Broadening Scenario

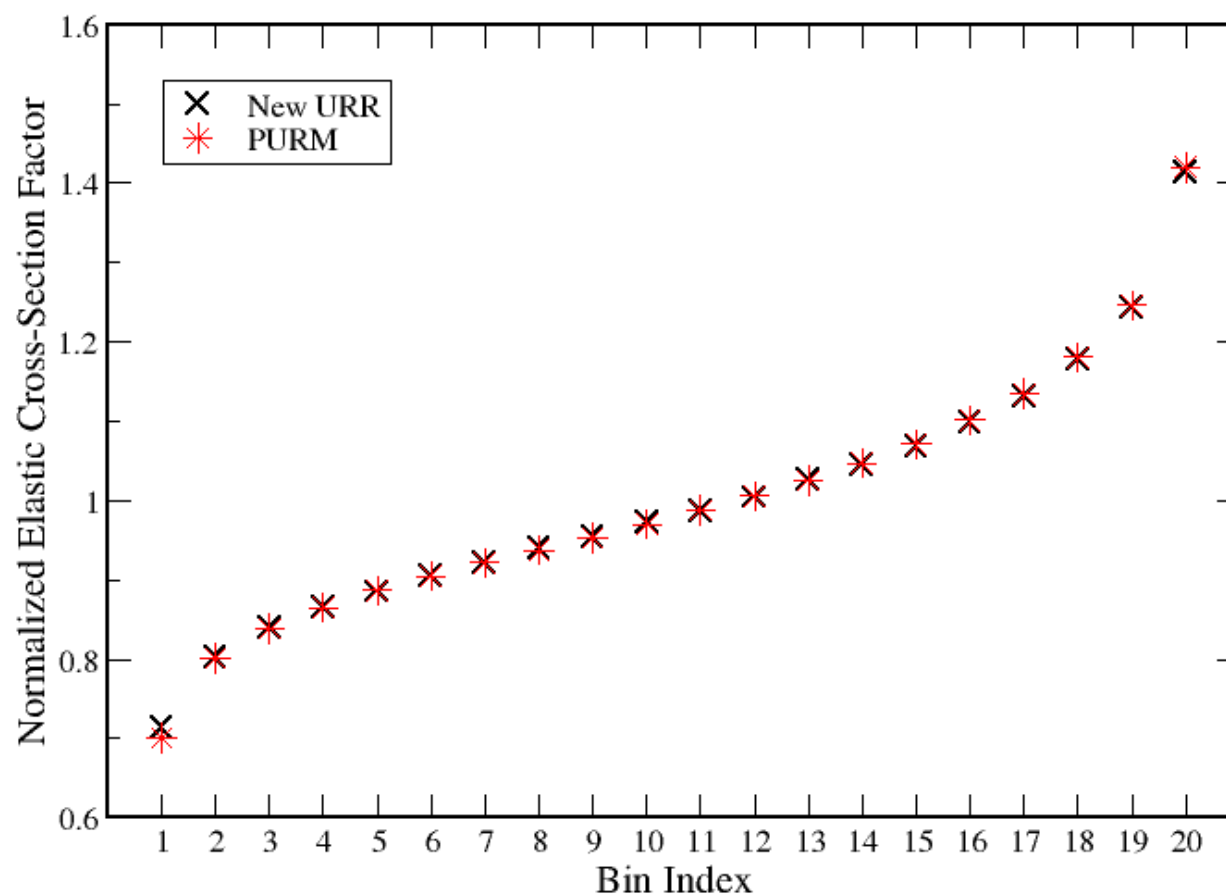


# Probability Table for $^{238}\text{U}$ at 140 keV and 293.6 K

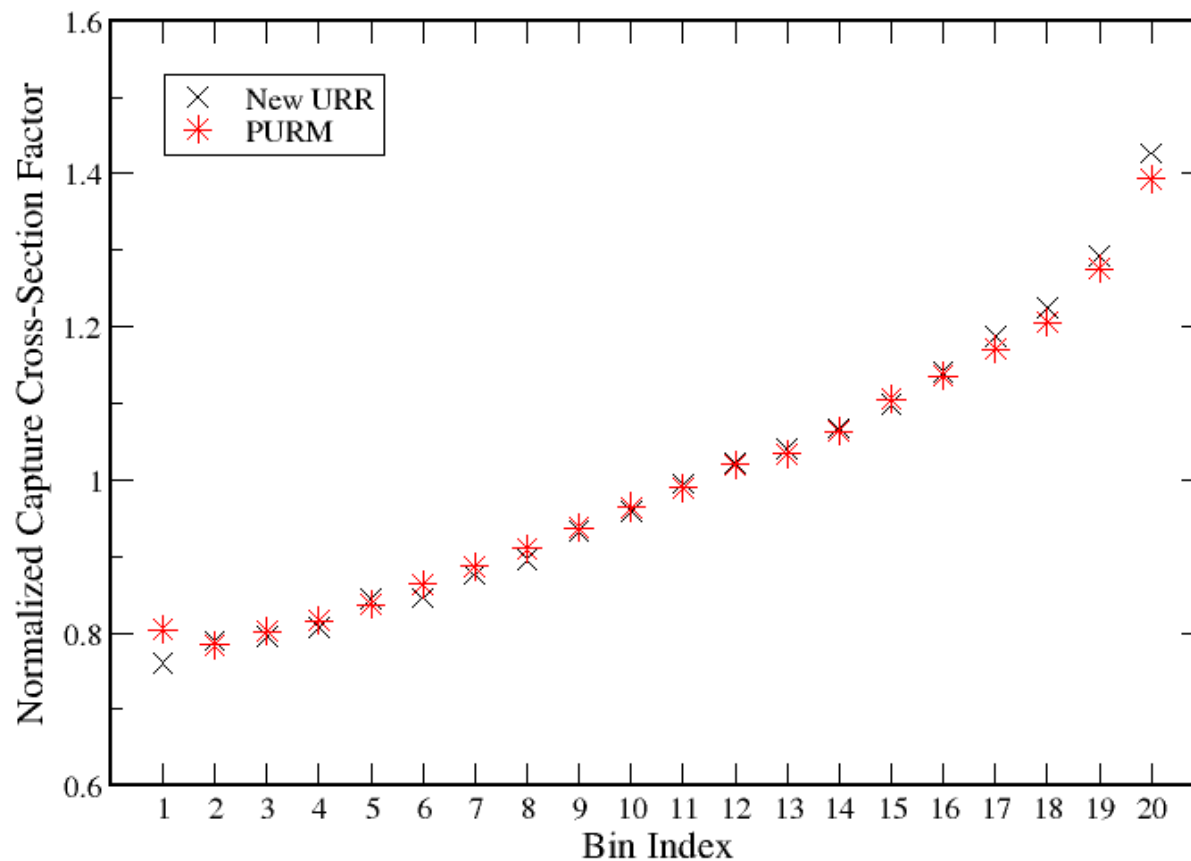
$^{238}\text{U}$  Normalized Total Cross-Section Factors at 140keV and 293.6K



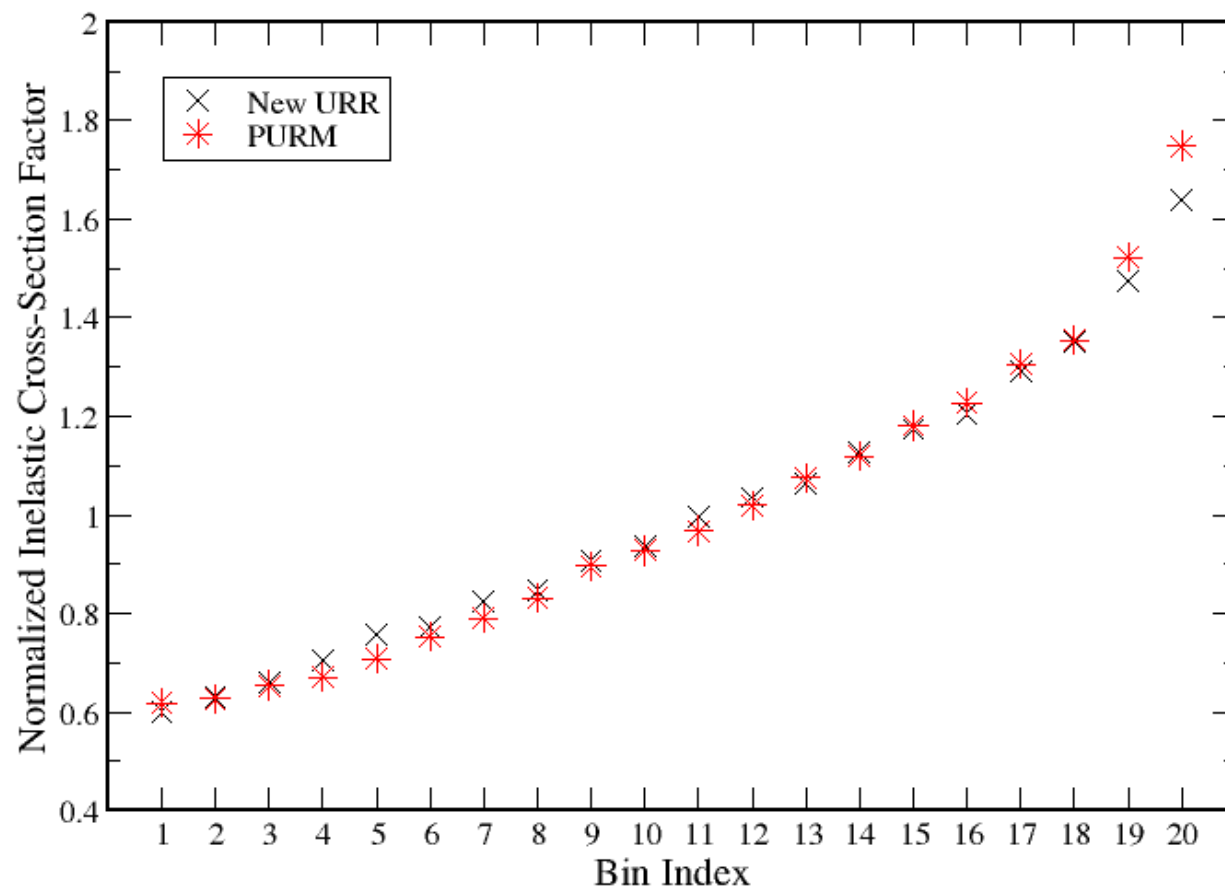
$^{238}\text{U}$  Normalized Elastic Cross-Section Factors at 140keV and 293.6K



$^{238}\text{U}$  Normalized Capture Cross-Section Factors at 140keV and 293.6K



$^{238}\text{U}$  Normalized Inelastic Cross-Section Factors at 140keV and 293.6K



# Benchmark Problems

- Benchmark problems run using MCNP ENDF/BVII.0 libraries and ENDF/BVII.1 libraries [9]
  - Modified  $^{238}\text{U}$  library by overwriting probability tables with new results
- Benchmarks – chosen for  $^{238}\text{U}$  sensitivity [10]
  - IEU-MET-FAST-007 (Big Ten)
  - IEU-MET-FAST-003 (bare sphere)
  - IEU-COMP-FAST-004 (ZPR-3 Assembly 12)

# IEU-MET-FAST-007 Results

Library	Probability Tables	MCNP5v1.6	MCNP6.1
Benchmark			$1.0049 \pm 0.0008$
ENDF/BVII.0	No	$1.00098 \pm 0.00007$	$1.00098 \pm 0.00007$
ENDF/BVII.0	Yes	$1.00492 \pm 0.00008$	$1.00492 \pm 0.00008$
ENDF/BVII.0+Modified <sup>238</sup> U	No	$1.00098 \pm 0.00007$	$1.00098 \pm 0.00007$
ENDF/BVII.0+Modified <sup>238</sup> U	Yes	$1.00537 \pm 0.00007$	$1.00537 \pm 0.00007$
ENDF/BVII.1	No	$1.00089 \pm 0.00007$	$1.00089 \pm 0.00007$
ENDF/BVII.1	Yes	$1.00453 \pm 0.00007$	$1.00453 \pm 0.00007$
ENDF/BVII.1+Modified <sup>238</sup> U	No	$1.00089 \pm 0.00007$	$1.00089 \pm 0.00007$
ENDF/BVII.1+Modified <sup>238</sup> U	Yes	$1.00531 \pm 0.00007$	$1.00531 \pm 0.00007$

# IEU-MET-FAST-003 Results

Library	Probability Tables	$k_{eff}$
Benchmark		$1.0000 \pm 0.0017$
ENDF/BVII.1	No	$1.00266 \pm 0.00009$
ENDF/BVII.1	Yes	$1.00222 \pm 0.00009$
ENDF/BVII.1+Modified <sup>238</sup> U	No	$1.00266 \pm 0.00009$
ENDF/BVII.1+Modified <sup>238</sup> U	Yes	$1.00204 \pm 0.00009$

# IEU-COMP-FAST-004 Results

Library	Probability Tables	$k_{eff}$
Benchmark		$0.9982 \pm 0.0015$
ENDF/BVII.1	No	$0.99833 \pm 0.00008$
ENDF/BVII.1	Yes	$0.99995 \pm 0.00009$
ENDF/BVII.1+Modified $^{238}\text{U}$	No	$0.99833 \pm 0.00008$
ENDF/BVII.1+Modified $^{238}\text{U}$	Yes	$1.00052 \pm 0.00008$

# Conclusions and Future Work

- Developed a new URR methodology consistent with RRR treatment
  - RML algorithm rigorously tested for variety of isotopes
  - New  $^{238}\text{U}$  probability tables in good agreement with current standards
  - Demonstrated excellent agreement with several  $^{238}\text{U}$ -sensitive benchmark problems
- Moving forward...
  - Code parallelization
  - Investigate sensitivity to energies of reference
  - Other isotopes, problems

# Acknowledgement

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# References

- [1] TRKOY, A., HERMAN, M., and BROWN, D., "ENDF-6 Formats Manual," tech. rep., Report BNL-90365-2009 Rev. 2, Brookhaven National Laboratory, Upton, New York, 2011.
- [2] FODERARO, A., *The Elements of Neutron Interaction Theory*, MIT Press, 1971.
- [3] LARSON, N. M., MOXON, M. C., LEAL, L. C., and DERRIEN, H., "Doppler Broadening Revisited," ORNL/TM-13525, Oak Ridge National Laboratory, 1998.
- [4] D. Wiarda, M. L. Williams, C. Celik, and M. E. Dunn, "AMPX: A Modern Cross-Section Processing System For Generating Nuclear Data Libraries," ICNC 2015, Charlotte, North Carolina, September 13–17, 2015.
- [5] DUNN, M. E. and LEAL, L. C., "Calculating Probability Tables for the Unresolved-Resonance Region Using Monte Carlo Methods," Proceedings of the International Conference on the New Frontiers of Nuclear Technology: Reactor Physics, Safety and High Performance Computing (PHYSOR 2002), Seoul, Korea, October 7-10, 2002.
- [6] LEAL, L. C. and HWANG, R., "A Finite Difference Method for Treating the Doppler Broadening of Neutron Cross Sections," in *American Nuclear Society*, (Los Angeles, CA), Nov. 1987.
- [7] HART, S. W. D., "Automated Doppler Broadening of Cross Sections for Neutron Transport Applications. " PhD diss., University of Tennessee, 2014. [http://trace.tennessee.edu/utk\\_graddiss/3136](http://trace.tennessee.edu/utk_graddiss/3136)
- [8] DUNN, M. E. and GREENE, N. M. "POLIDENT: A Module for Generating Continuous-Energy Cross Sections from ENDF Resonance Data," ORNL/TM-2000-035, Oak Ridge National Laboratory, 2000.
- [9] T. Goorley, et al., "Initial MCNP6 Release Overview", Nuclear Technology, **180**, pp 298-315 (Dec 2012).
- [10] "INTERNATIONAL HANDBOOK OF EVALUATED CRITICALITY SAFETY BENCHMARK EXPERIMENTS," NEA/NSC/DOC(95)03/I-VIII, OECD-NEA, September, 2004.